Parallel H-Adaptivity Applications in the ALEGRA Code

Michael Wong

Randy Weatherby

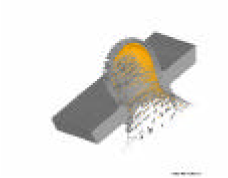
Ed Boucheron

Computational Physics Department

Sandia National Laboratories*

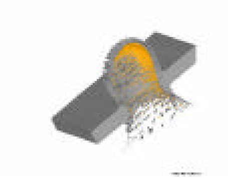
***Sandia is a multi-program laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.**

Sandia National Laboratories



Introduction

- **Overview**
- **H-Adaptivity Implementation**
  - **Topology and Data Structures**
  - **Parallelization**
  - **Error Metrics**
  - **Load Balancing**
- **Current Research and Issues**
- **Conclusions**

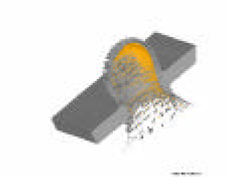


Overview: ALEGRA

Computational Physics R&D Department

- **ALEGRA is a strong shock wave and coupled physics code designed to solve high strain rate, high energy, problems.**
- **Customers**
  - Sandia Pulsed Power Research
  - Sandia Computational Physics
  - DoD Applications
  - DoE Defense Program
- **Some Features**
  - 2D/3D Geometries
  - Lagrangian Physics (Pronto kernel)
  - Multi-Material Arbitrary-Lagrangian-Eulerian (ALE) Physics
  - H-Adaptivity
  - Massively Parallel Architecture
  - Variety of Material Models and Flexible Interface

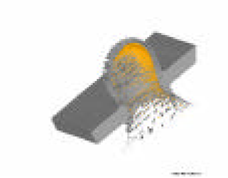
Sandia National Laboratories



Overview: H-Adaptivity

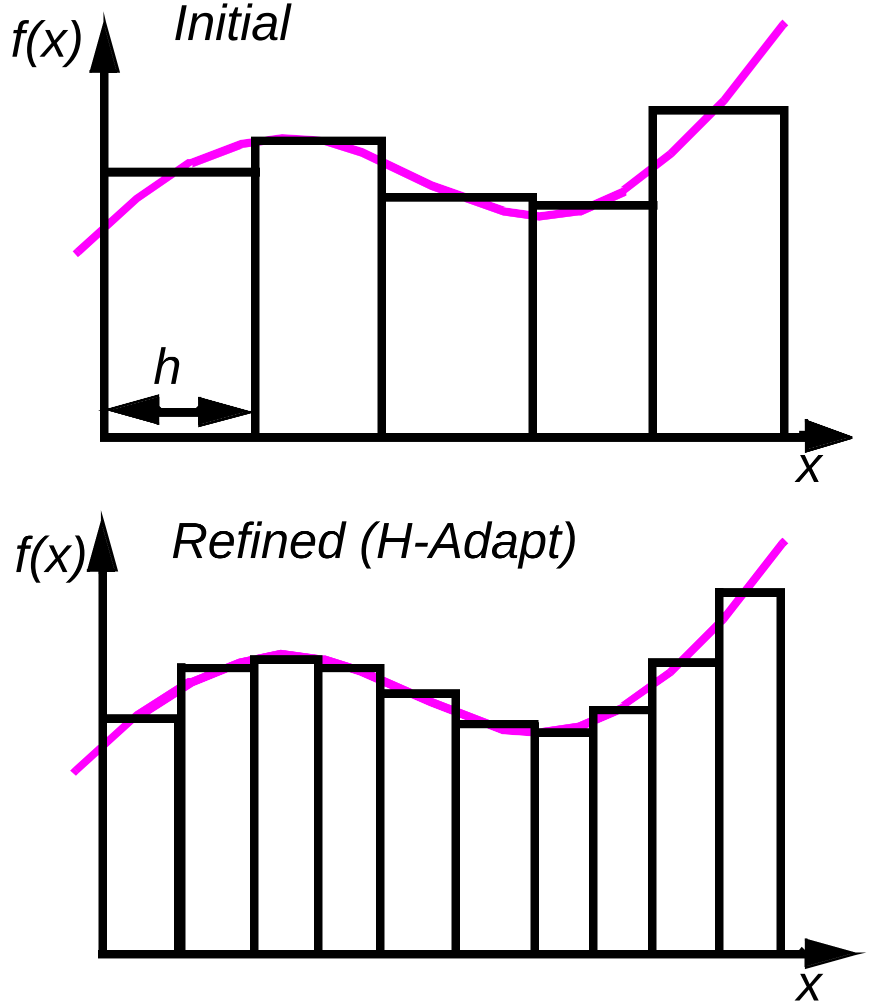
- **Objective: to provide efficient, <u>high precision</u> simulation capabilities for ALEGRA through flexible, robust h-adaptivity of finite elements.**
  - Efficiency: Use less memory, less computational time than a non-refining mesh providing the same maximum resolution.
  - High Precision: Provide fine, highly resolved mesh where and when such precision is needed.
  - Provide new and unique capabilities which augment spatial discretization (e.g., initial mesh refinement, arbitrary mesh creation).
- **Critical technologies for H-Adaptivity**
  - Dynamic Load Balancing
  - Parallelization of Adaptivity
  - Error Measurement and Refinement Drivers

Sandia National Laboratories

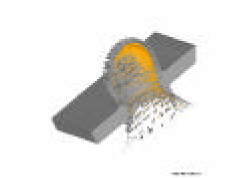


Adaptivity Concept

– **<u>H-Adaptivity</u>: *refinement* of finite element mesh by increasing the number of elements (changing *h*, characteristic element size)**

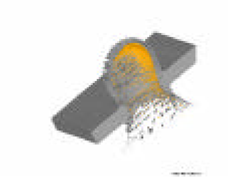


Sandia National Laboratories



Motivations

- **Spatial resolution requirements of the largest problems will exceed the available computing resources for the foreseeable future.**
- **Selective high resolution regions necessary but only for small periods of time.**
- **Multiple and different computing platforms and architectures expected.**
- **Current platforms:**
  - Workstations (SUN, HP, SGI, IBM) / OS's (Solaris, HPUX, IRIX, AIX, OSF/1)
  - Clusters (SGI Origin2000, DEC, Cplant)
  - Supercomputer (ASCI Red, Pacific Blue, Mountain Blue)

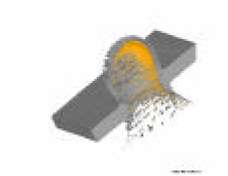


H-Adaptivity Implementation

- **Data Structures**
  - **Topological Entities: Element, Face, Edge, Vertex**

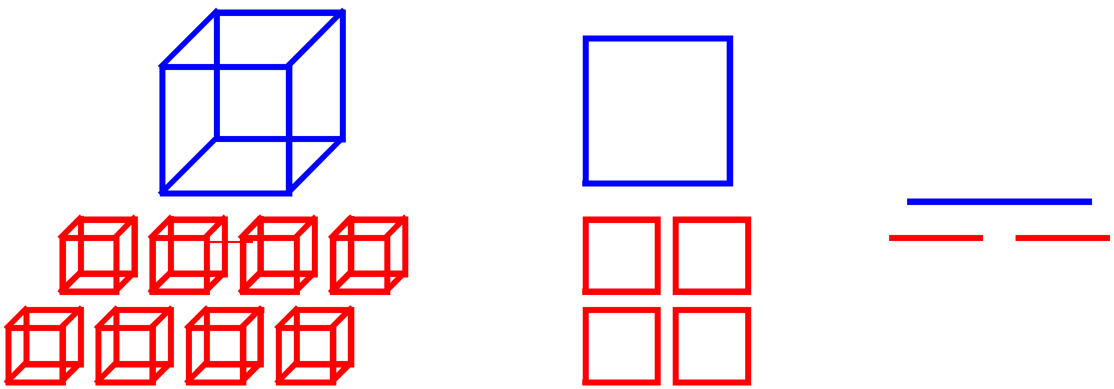
Entity *(Vertex | Edge | Face | Element)*	
Data:	**Functions:**
Variable Data	**Geometry (length, volume, etc)**
Material Data	**Calculus (grad, integral, etc)**
Attributes	**Adaptivity (refine/unrefine,split/join)**
Connectivity pointers	**Connectivity & Attribute access**
Genealogy pointer	

  - **All data and functionality contained in entity: departs from traditional array based storage; storage in cache-sized chunks.**
  - **Entities contain only variables *registered* at runtime, by the physics algorithms**

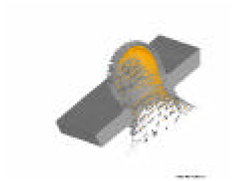


H-Adaptivity Implementation

- **Data Structures (continued)**
  - **Linked Lists for managing entities in the algorithms**
    - » **Replaces traditional DO loop of array-based codes**
    - » **Currently links all active entities**
    - » **Linked List for collection of local and ghost entities.**
    - » **Additional lists created as needed on a temporary basis**
  - **Geneaological Trees for managing refinement paths**
    - » **Tree structure used to relate parent object to children.**
    - » **The breadth of the tree depends on the specific object.**
    - » **All objects (except Vertex) are capable of parent-child relationship.**

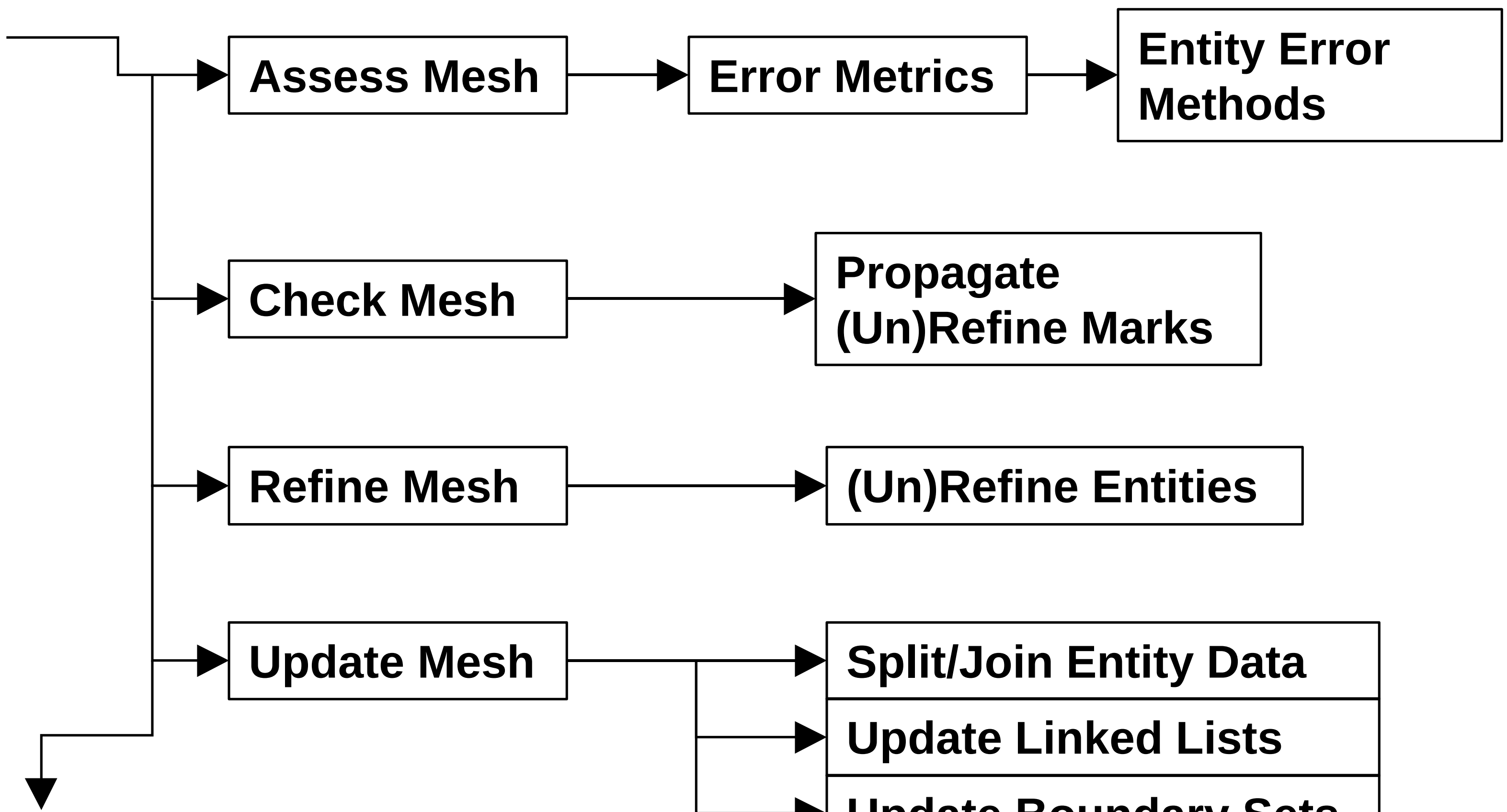


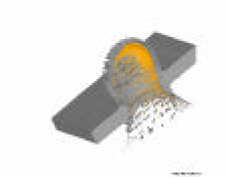
Hex8 Quad4 or Quad4Face Edge



H-Adaptivity Implementation

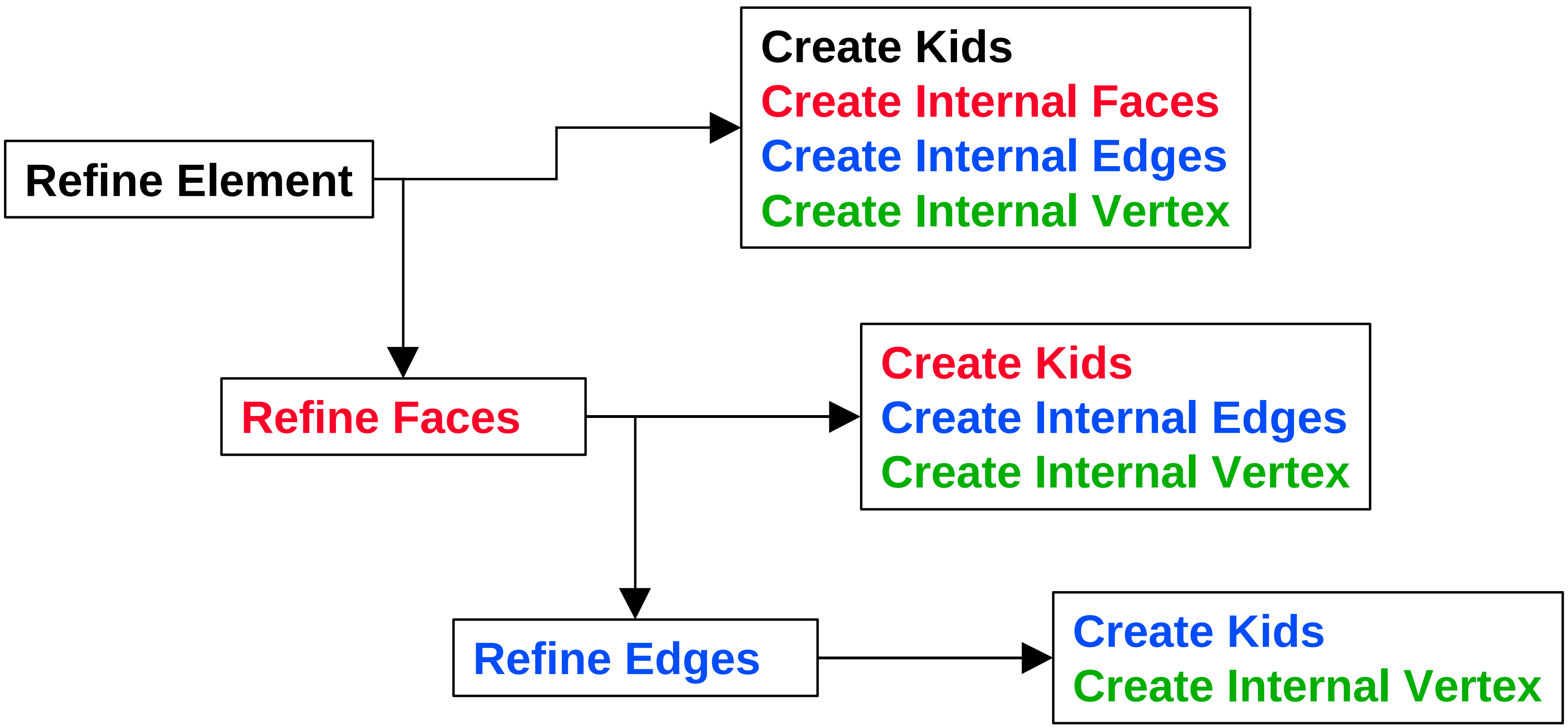
- **Adaptivity Control**

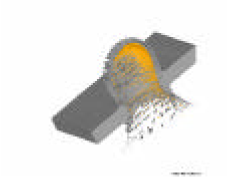




H-Adaptivity Implementation

- **Refinement/Unrefinement of Elements**
  - template approach: refinement of an element produces specific entities with specific connectivities.



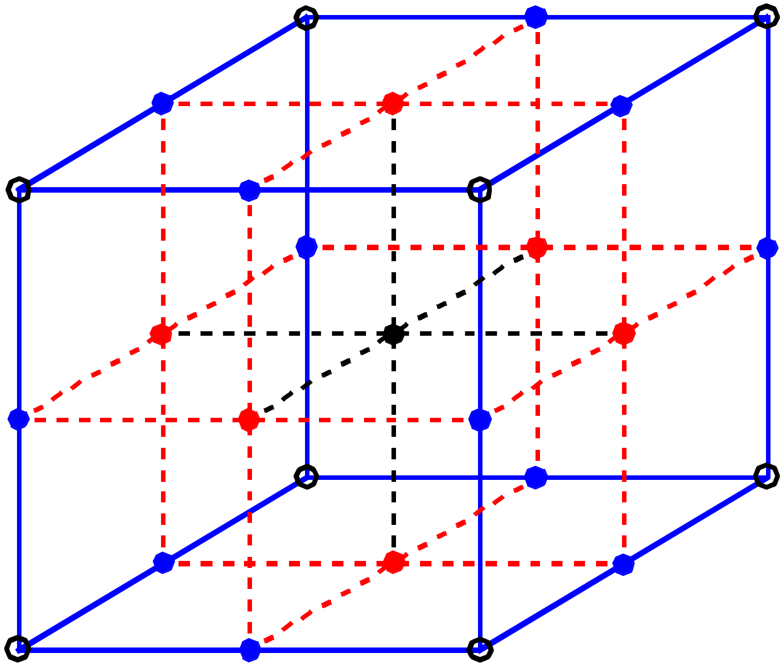


H-Adaptivity Implementation

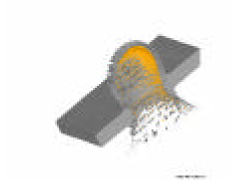
Computational Physics R&D Department

- **Refinement/Unrefinement of Elements**

ENTITY	PARENT	REFINED	KIDS	CREATED	SPLIT
Element	1	8	8	0	8
Face	6	36	4	12	24
Edge	12	54	2	(face) 24 (internal) 6	24
Vertex	8	27	0	(edge) 12 (face) 6 (internal) 1	0

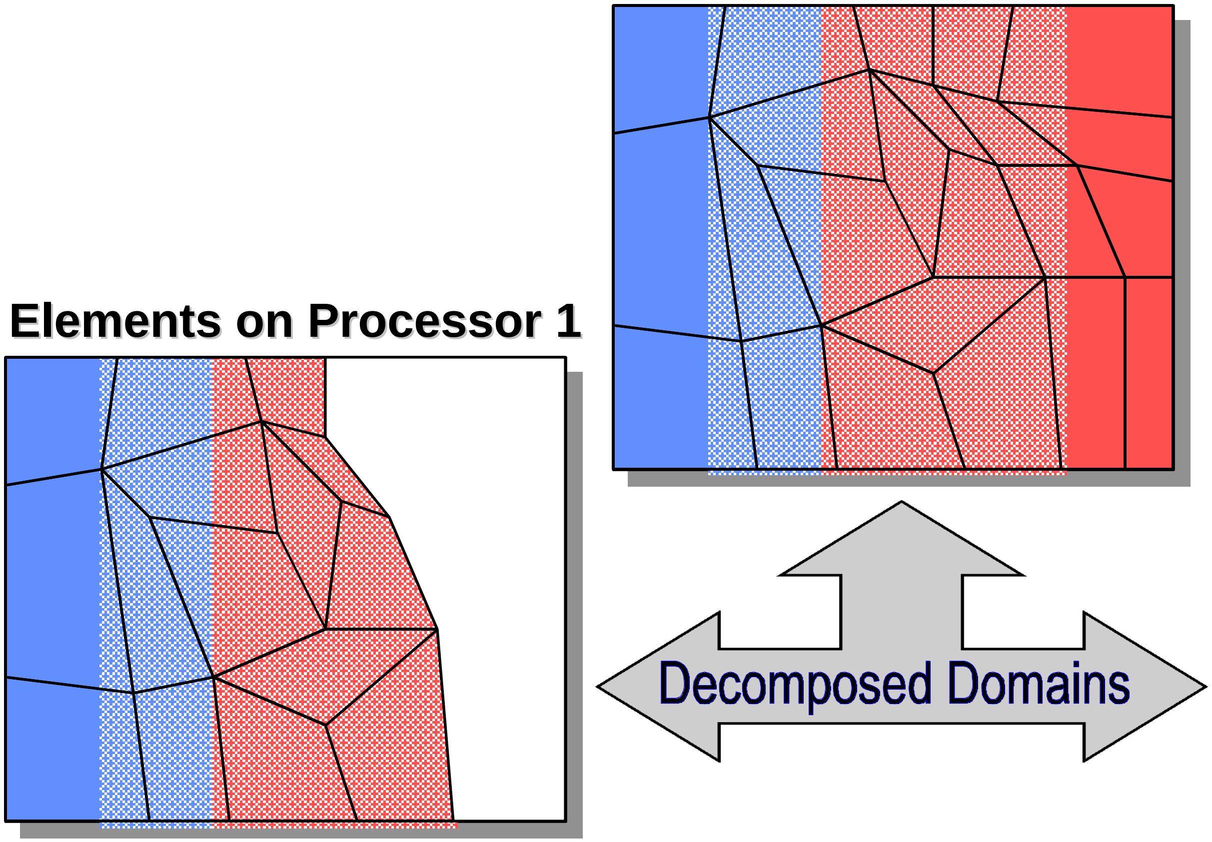


Sandia National Laboratories



Domain Decomposition in ALEGRA

Computational Physics R&D Department



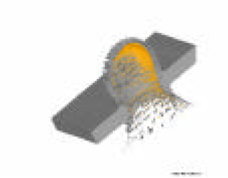
Processor 1:

- Local elements
- Local elements on processor boundary
- Ghost elements

Processor 2:

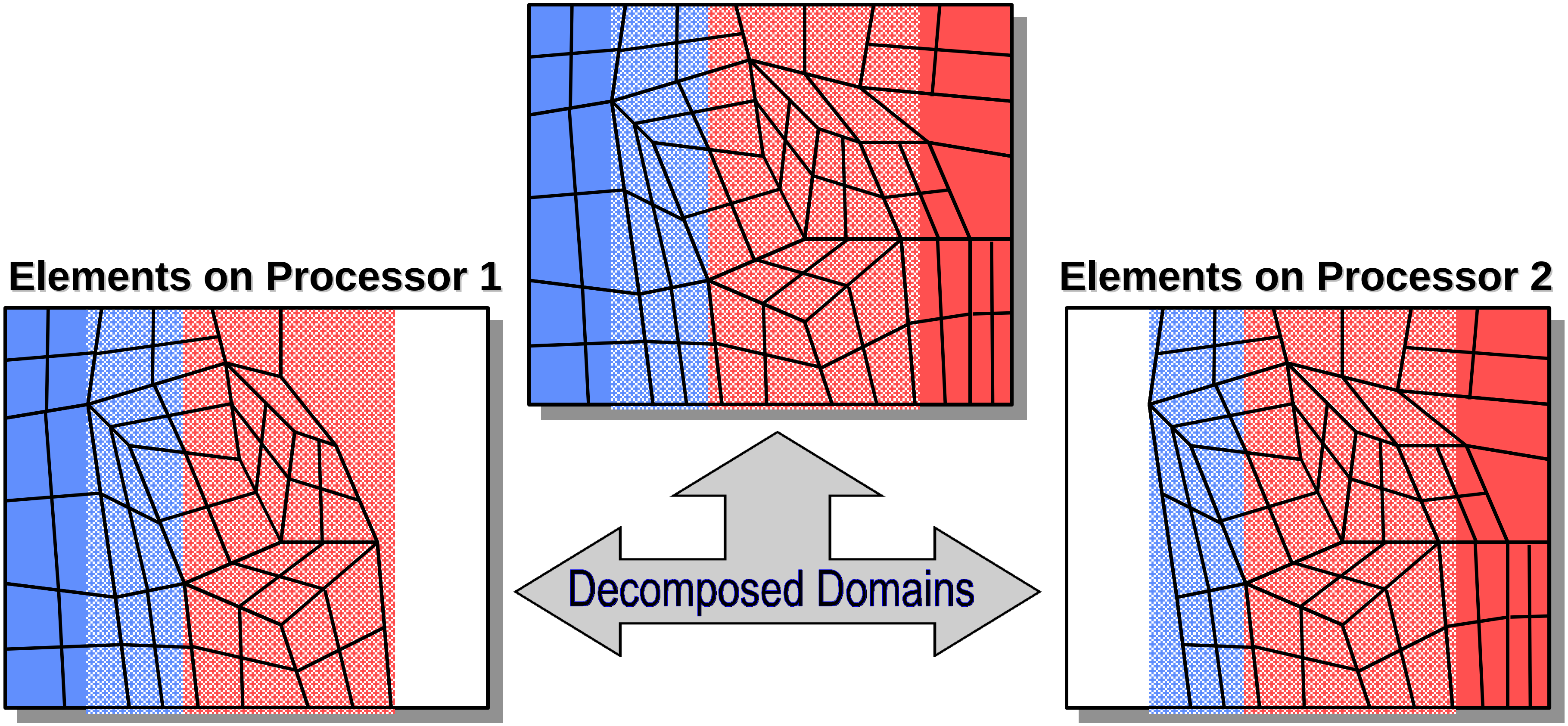
- Local elements
- Local elements on processor boundary
- Ghost elements

Sandia National Laboratories



First Stage of Parallel Adaptivity

Computational Physics R&D Department



Processor 1 legend:

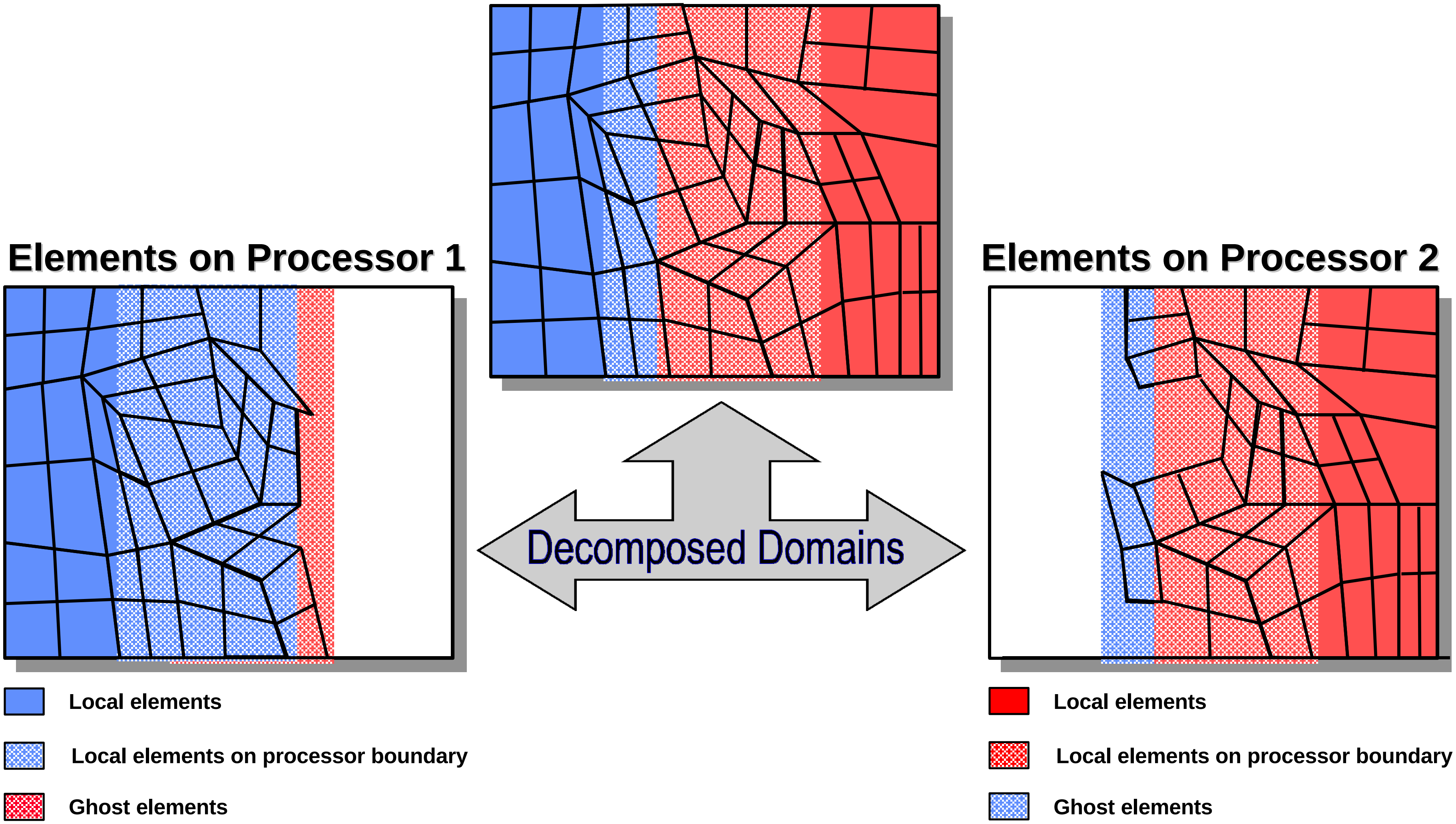
- **Local elements**
- **Local elements on processor boundary**
- **Ghost elements**

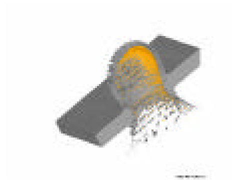
Processor 2 legend:

- **Local elements**
- **Local elements on processor boundary**
- **Ghost elements**

Second Stage of Parallel Adaptivity

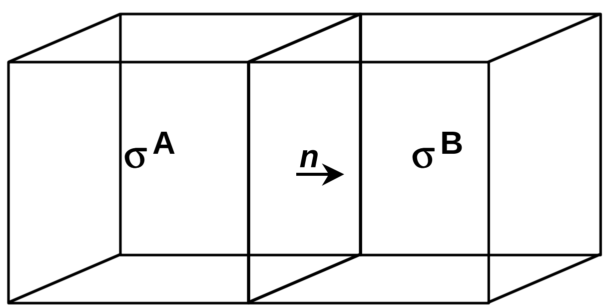
Computational Physics R&D Department





Error Metric Interface

- **Objectives:**
  - flexible implementation interface
  - testbed for development and evaluation of error drivers, indicators, and estimators
  - allow for modular and composite error metrics to accommodate coupled physics
- **Currently available metric - Jump Error**

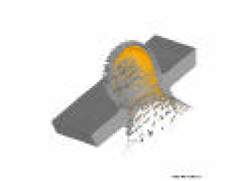


$$err = \left\| \left(s^{A} - s^{B} \right) \cdot n \right\|$$

err > rT, refine
err < uT, unrefine

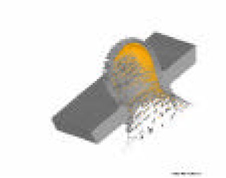
r, u, T - user parameters

Sandia National Laboratories



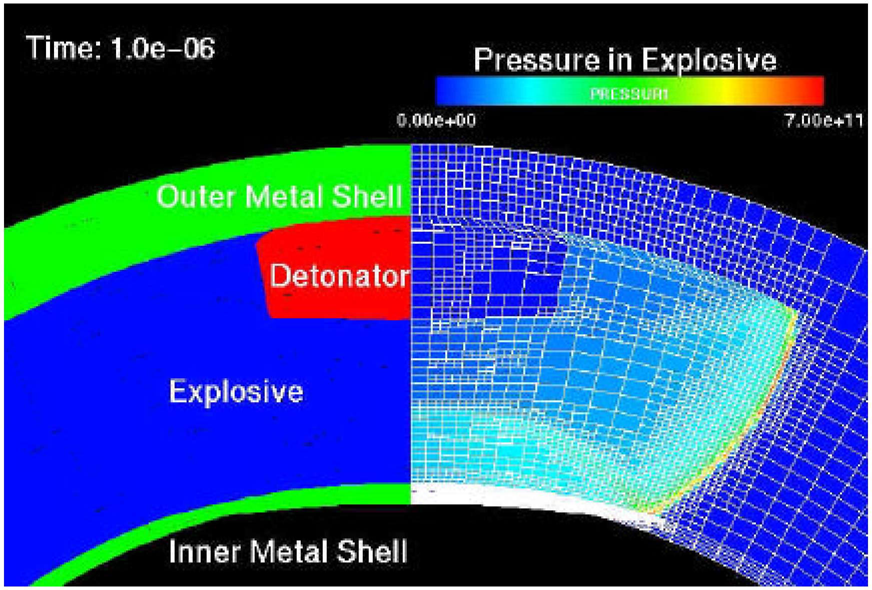
Dynamic Load Balancing Approaches

- **Why Dynamic Load Balancing?**
  - » Five levels of adaptive refinement can multiply hex elements on a processor by a factor of 32768
  - » Load imbalance forecast factors of 10-1000 are credible
- **Possible Load Balancing Approaches**
  - » atomic - move single elements at will
  - » layer - “peel” layers of elements off processor
  - » ancestor - move ancestor and all children
  - » full rebalance - generate new domain decomposition
- **Current Status**
  - » Basic processor load information implemented
  - » Logic for “peeling” layers of elements implemented
  - » Movement methods developed that retain connectivity information and reconstruct topological entities on new processor
  - » Implementing remesh strategy with external library in development



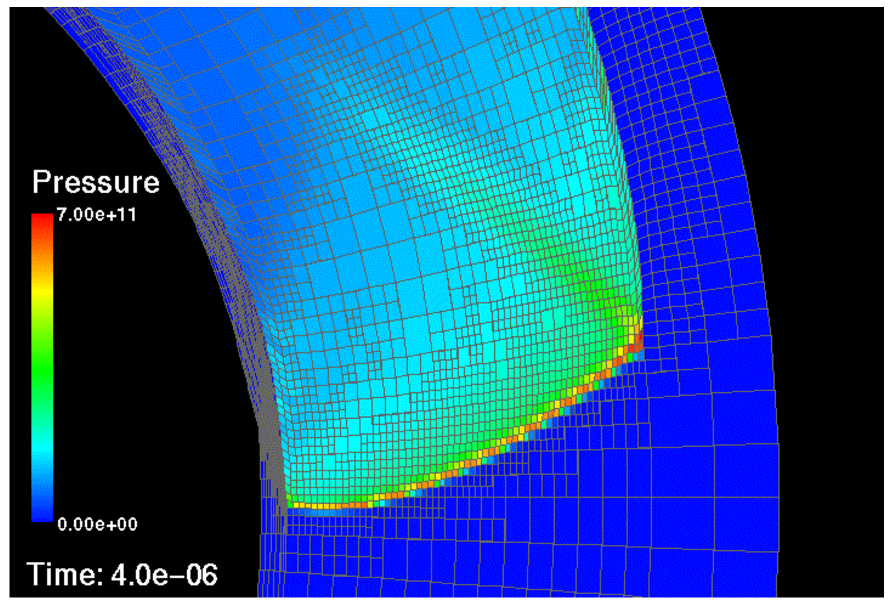
Current Status - Example

Computational Physics R&D Department

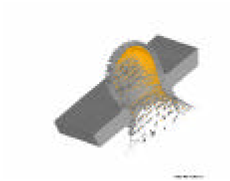


- **Explosive sandwiched between two metal shells (elastic-plastic)**
- **Reactive burn explosive materials**
- **Used Jump Error as Error Metric**

- **Run on 8 processors**
- **Limited to two levels of refinement**
- **Pressure painted by element**

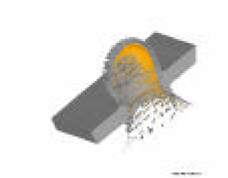


Sandia National Laboratories



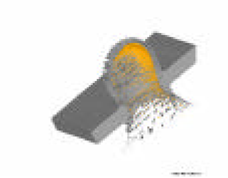
Current Research and Issues

- **Large-Scale MP Shock Simulation (Tera-scale)**
  - mechanical shock wave simulations requiring adaptivity to support SBSS in ASCI
- **H-Adaptivity with Advection**
  - currently H-Adaptivity is limited to Lagrangian meshes
  - extending the H-Adaptivity capability to work with Advection allows H-Adaptivity to work on Eulerian or ALE meshes.
- **Robust and Efficient Error Indicators for Shock Propagation**
  - currently working to populate models derived from the Error_Metric class.
  - experimenting with published error indicator/estimator techniques
  - generalizing the Jump_Error to accommodate other variables and norms



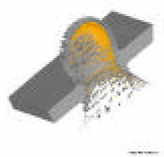
Current Research and Issues

- **Robust Adapting of Variable Data**
  - projection of variable data between levels is generally simplistic
    - » copy value from parent to children during refinement
    - » average value from children to parent during unrefinement
    - » specialized methods for selected variables (e.g., node_mass)
  - currently do not address variables that have history and are dependent on element dimensions
    - » hourglass control
- **Robust and Efficient Dynamic Load Balancing**
  - aggressiveness of adaptivity is limited by the capability to perform efficient dynamic load balancing
  - currently integrating the basic load balancing methods with the parallel adaptive capability



Current Research and Issues

- **Integration of Adaptivity with Non-mechanics Physics**
  - **extend adaptive capability to electro-mechanical solutions**
    - » **electric field solution is implicit (a posteriori error estimates possible)**
    - » **hydrodynamics solution is explicit (I.e., use jump error)**
    - » **need to properly interface with linear solver package to accommodate adapted meshes**
  - **leverage adaptivity topology architecture to support multigrid or multilevel iterative solvers.**



Conclusion

- **Current Status of Adaptivity**
  - 2D/3D H-Adaptivity
  - Lagrangian meshes
  - Parallel 2D/3D
  - Basic dynamic load balancing
  - Solid dynamics physics
- **Work in Progress**
  - Large-Scale MP-Computing
  - Algorithm development continuing